kinetics, and undercooling. The method is based on two ideas. First, the equations of motion are recast as a single history-dependent boundary integral equation on the solid/liquid boundary. A fast algorithm is used to solve the integral equation efficiently. Second, the boundary is moved by solving a "Hamilton–Jacobi"-type equation (on a *fixed* domain) formulated by Osher and Sethian for a function in which the boundary is a particular level set. This equation is solved by finite difference schemes borrowed from the technology of hyperbolic conservation laws. The two ideas are combined by constructing a smooth extension of the normal velocity off the moving boundary, in a way suggested by the physics of the problem. Our numerical experiments show the evolution of complex crystalline shapes, development of large spikes and corners, dendrite formation and side-branching, and pieces of solid merging and breaking off freely.

AN EVALUATION OF THE SNIFFER GLOBAL OPTIMIZATION ALGORITHM USING STANDARD TEST FUNCTIONS. Roger A. R. Butler and Edward E. Slaminka. *Mathematics Department, Auburn University, Auburn, Alabama 36849-5310, USA.*

The performance of Sniffer—a new global optimization algorithm—is compared with that of Simulated Annealing. Using the number of function evaluations as a measure of efficiency, the new algorithm is shown to be significantly better at finding the global minimum of seven standard test functions. Several of the test functions used have many local minima and very steep walls surrounding the global minimum. Such functions are intended to thwart global minimization algorithms.

ORTHOGONAL MAPPING IN TWO DIMENSIONS. Ramani Duraiswami and Andrea Prosperetti. *Department of Mechanical Engineering, 127 Latrobe Hall, The Johns Hopkins University, Baltimore, Maryland 21218, USA.*

A method for the generation of orthogonal boundary-fitted curvilinear coordinates for arbitrary simply- and doubly-connected domains is developed on the basis of the theory of quasi-conformal mappings of quadrilaterals and of previous work by Ryskin and Leal. The method has useful applications in orthogonal grid generation in two-dimensional and axi-symmetric domains and in the extension of rapid elliptic solvers and spectral methods to complex geometries. A new technique for the calculation of the conformal module of quadrilaterals is also presented.

NUMERICAL INTEGRATION FOR POLYATOMIC SYSTEMS. G. te Velde and E. J. Baerends. *Afdeling Theoretische Chemie, Scheikundig Laboratorium der Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands.*

A numerical integration package is presented for three-dimensional integrals occurring in electronic structure calculations, applicable to all polyatomic systems with periodicity in 0 (molecules), 1 (chains), 2 (slabs), or 3 dimensions (crystals). The scheme is cellular in nature, based on Gaussian product formulas and it makes use of the geometrical symmetry. Convergence of accuracy with the number of points is rapid and use of the program has been made easy.

A NUMERICAL METHOD FOR SOLVING SYSTEMS OF LINEAR ORDINARY DIFFERENTIAL EQUATIONS WITH RAPIDLY OSCILLATING SOLUTIONS. Ira B. Bernstein. *Department of Applied Physics, Yale University, Yale Station, New Haven, Connecticut 06520-2159, USA, and Center for Solar and Space Research, Yale University, P.O. Box 6666, New Haven, Connecticut 06511-6666, USA*; Leigh Brookshaw. *Department of Applied Physics, Yale University, Yale Station, New Haven, Connecticut 06520-2159, USA*; Peter A. Fox. *Center for Solar and Space Research, Yale University, P.O. Box 6666, New Haven, Connecticut 06511-6666, USA.*

A numerical method is presented which allows the accurate and efficient solution of systems of linear equations of the form $dz_i(x)/dx = \sum_{j=1}^{N} A_{ij}(x)\, z_j(x)$, $i = 1, 2, ..., N$, when the solutions vary rapidly compared with the $A_{ij}(x)$. The method consists of numerically developing a set of basis solutions characterized by new dependent variables which are slowly varying. These solutions can be accurately computed with an overhead that is substantially independent of the smallness of the scale length characterizing the solutions. Examples are given.

THE ASYMPTOTIC DIFFUSION LIMIT OF A LINEAR DISCONTINUOUS DISCRETIZATION OF A TWO-DIMENSIONAL LINEAR TRANSPORT EQUATION. Christoph Börgers. *Department of Mathematics, University of Michigan, Ann Arbor, Michigan 48109, USA*; Edward W. Larsen. *Department of Nuclear Engineering, University of Michigan, Ann Arbor, Michigan 48109, USA*; Marvin L. Adams. *Lawrence Livermore National Laboratory, University of California, Livermore, California 94550, USA.*

Consider a linear transport problem, and let the mean free path and the absorption cross section be of size ε. It is well known that one obtains a diffusion problem as ε tends to zero. We discretize the transport problem on a fixed mesh, independent of ε, consider again the limit $\varepsilon \to 0$, and ask whether one obtains an accurate discretization of the continuous diffusion problem. The answer is known to be affirmative for the linear discontinuous Galerkin finite element discretization in one space dimension. In this paper, we ask whether the same result holds in two space dimensions. We consider a linear discontinuous discretization based on rectangular meshes. Our main result is that the asymptotic limit of this discrete problem is *not* a discretization of the asymptotic limit of the continuous problem and thus that the discretization will be inaccurate in the asymptotic regime under consideration. We also propose a modified scheme which has the correct asymptotic behavior for spatially periodic problems, although not always for problems with boundaries. We present numerical results confirming our formal asymptotic analysis.

HYDRODYNAMIC MODELING OF PARTICLE AND ANGULAR MOMENTUM TRANSPORT IN ROTATING TOKAMAK PLASMAS WITH IMPURITIES. R. Zanino. *Energetics Department, Polytechnic Institute of Turin, Italy.*

We have developed a 1 + 1 D time dependent code for the description of ion-impurity transport in a rotating tokamak plasma, using a pseudo-spectral discretization in the poloidal angle θ and a staggered finite difference mesh in the minor radius r. The plasma is assumed to have a constant uniform temperature T, to be in the high collisionality (Pfirsch–Schlüter) regime, and to contain electrons "e," fuel ions "i," and a single impurity species "Z" of charge eZ, where e is the proton charge. We are particularly interested in the case when: (1) flow velocities in the toroidal (symmetry) direction ϕ are in the range typical of neutral beam injection experiments, i.e., $v_{thZ} < V_{\phi i,Z} \lesssim v_{thi}$, ($v_{thj} \equiv \sqrt{2T/m_j}$ is the thermal speed, m_j is the mass); (2) the relative concentration of impurities in the plasma, $\bar{n}_Z/\bar{n}_i$, is significant and comparable to that observed in present tokamaks, i.e., $\sqrt{m_e/m_i} \ll \bar{n}_Z Z^2/\bar{n}_i \approx 1$ in order of magnitude. The model fluid equations are obtained via a moment approach, and an expansion in powers of the small ordering parameter $\delta_{pi} \equiv (m_i v_{thi}/e\mathbf{B}_\theta)((1/\bar{n}_i)\,|\,\partial\bar{n}_i/\partial r|) \ll 1$ ($\mathbf{B}$ is the magnetic field) is then employed. The equations at each order in δ_{pi} up to the second are solved, and the characteristic features of the results presented: to lowest order, outboard impurity peaking on each magnetic surface appears due to centrifugal forces; to first order, radial gradients driven ion-impurity friction gives rise to up–down asymmetries in

the poloidal profiles; to second order, the radial profiles of density and rotation frequency evolve to steady state under the action of particle and angular momentum sources. The evolution of the poloidal profiles is decoupled from the evolution of the radial ones, thanks to the fact that the corresponding time scales belong to different orders in δ_{pi}: an algorithm is proposed to treat the 2D problem, alternating the solution of 1D problems.

TIME-IMPLICIT FLUID SIMULATION OF COLLISIONAL PLASMAS. P. W. Rambo and J. Denavit. *University of California, Lawrence Livermore National Laboratory, Livermore, California 94550, USA.*

A one-dimensional algorithm for fluid simulation of interpenetrating multi-component plasmas, developed earlier for the collisionless case, is extended to include collisions between species. The finite- differenced fluid equations, including collision forces, are coupled with the Poisson equation to give time-implicit solutions, which are stable and accurate over a wide range of the time scale parameters $\omega_p \Delta t$ and $\nu_c \Delta t$ (ω_p is the plasma frequency, ν_c is a typical collision frequency, and Δt is the time step). In regions where $\omega_p \Delta t \ll 1$ and $\nu_c \Delta t \ll 1$, electron dynamics and space-charge effects are resolved, while in regions where $\omega_p \Delta t \gg 1$ and/or $\nu_c \Delta t \gg 1$, the ambipolar and/or diffusion models are recovered. Results of tests are presented, including ohmic heating, shocks with an interface between different fluids, colliding plasmas in which a region of interpenetrating fluids is created, and plasma shocks with separate electron and ion fluids.

AN ALGORITHM FOR THE SOLUTION OF INVERSE LAPLACE PROBLEMS AND ITS APPLICATION IN FLAW IDENTIFICATION IN MATERIALS. Shuvra Das and Ambar K. Mitra. *Department of Engineering Science and Mechanics, Iowa State University, Ames, Iowa 50011, USA.*

An algorithm for solving an inverse problem in steady state heat conduction is developed. In this problem, the location and shape of the inner boundary of a doubly connected domain is unknown. Instead, additional experimental data are provided at several points on the outer boundary. Through an iterative process, the unknown boundary is determined by minimizing a functional. Convergence properties of the algorithm are examined, and the stopping criterion for the iterative process is developed from numerical experiments in a simple case. The scheme is shown to perform well for the complex case of an L-shaped crack in a square domain.

NUMERICAL ANALYSIS OF 2D MHD EQUILIBRIUM WITH NON-INDUCTIVE PLASMA CURRENT IN TOKAMAKS. K. Tani and M. Azumi. *Japan Atomic Energy Research Institute, Naka-machi, Naka-gun, Ibaraki-ken, Japan 311-01*; R. S. Devoto. *Lawrence Livermore National Laboratory, P.O. Box 5511, Livermore, California 94550, USA.*

We have developed a numerical code to investigate steady state neutral-beam-driven, ohmic and bootstrap currents which are consistent with MHD equilibrium. The code can describe the effects of mirror trapping, energy diffusion, and bounce motion of fast ions on the beam-driven current. The bootstrap current is evaluated for multi-species ions including impurity and unthermalized fast ions. An iterative algorithm is employed to obtain a self-consistent current and MHD equilibrium. MHD stability for the converged solution can also be investigated with the code.

A MULTIGRID CONJUGATE RESIDUAL METHOD FOR THE NUMERICAL SOLUTION OF THE HARTREE–FOCK EQUATION FOR DIATOMIC MOLECULES. Kjell Davstad. *Institute of Theoretical Physics, University of Stockholm, Vanadisvägen 9, S-113 46 Stockholm, Sweden.*

Discretization of the Hartree–Fock equations in operational form leads to unsymmetric positive definite and indefinite linear equations. To solve these equations a combination of the multigrid method and the Orthomin method with Gauss–Seidel relaxation as preconditioner is used. The differential equations are approximated to the sixth order and the solution is extrapolated to the eighth order. The method is fully parallelized. The largest molecule treated is CuH.

NOTE TO APPEAR

PARAMETERIZED SOLUTION OF ONE-DIMENSIONAL THERMAL DIFFUSION WITH A HEAT SOURCE AND A MOVING BOUNDARY. Edward J. Caramana and Robert B. Webster. *Group X-1; MS-E531, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA.*

Printed in Belgium